

Ising-like models on arbitrary graphs : The Hadamard way

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We propose a generic framework to describe classical Ising-like models defined on arbitrary graphs. The energy spectrum is shown to be the Hadamard transform of a suitably defined sparse "coding" vector associated with the graph. We expect that the existence of a fast Hadamard transform algorithm (used for instance in image compression processes), together with the sparseness of the coding vector may provide ways to fasten the spectrum computation. Applying this formalism to regular graphs, such as hyper cubic graphs, we obtain a simple recurrence relation for the spectrum, which significantly speeds up its determination. First attempts to analyze partition functions and transfer matrices are also presented.

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I. INTRODUCTION

Ising-like interactions enter paradigmatic sets of models defined to describe phase transitions in statistical physics, and has been applied to a very large set of a priori different problems, even outside physics. It is clearly not achievable to summarize in few words the many contributions on that subject, and the interested reader is referred to the numerous review papers or books, see for instance Ref.¹. Nevertheless useful to recall is the initial Ising-Lenz solution for the one-dimensional case², and the absence in that case of phase transition at positive temperature, the Peierls proof for the existence of a phase transitions in two dimensions³, followed later by the Onsager solution⁴. Up to now, and even though a large amount of work gives precise informations about the phase diagram in three dimensions, no exact solution is known in that case.

In this paper, we present an approach to address such models where classical two-level spins located at graph vertices interact through n-body terms (regular or disordered), which we generically call "Ising-like" models, the well known standard Ising model corresponding to one- and two-body interactions. We show how some simple algebraic tools can be used to describe and speed up the numerical solution of the spectral problem defined on an arbitrary graph. For sake of simplicity, we shall mainly concentrate our presentation on the standard Ising model, keeping in mind that most of what is said applies as well in the Ising-like cases. In a first step, we define a binary vector which fully describe the graph structure, and a "coding vector" which embodies the Hamiltonian. We then show that, under an Hadamard transformation, this coding vector is sent to a "spectral vector", whose components are the set full set of energies in the configuration space. An important point here is to recall the existence of a "Fast Hadamard Transform" (FHT), able in principle to considerably speed up the computation.

We then concentrate on some regular graphs (mainly hyper cubes), for which even stronger results can be derived. Finally, some preliminary attempts to adapt this formalism to transfer matrix and partition function determination will also be presented.

II. ISING-LIKE MODELS ON ARBITRARY GRAPHS

A. Ising-like Hamiltonian

We consider a graph G , with its N vertices gathered in a set V and its bonds, as pairs of neighboring vertices, in a set B . The simplest Ising model describes classical spins $S_i = \pm 1$ located at the G vertices, subject to a constant magnetic field h , and to constant pairwise interactions for spins connected by a graph edge. The spin configuration space is the product $(\pm 1)^{\otimes N}$, forming a hyper cube Γ_N in N dimensions, with its $M = 2^N$ vertices encoding the possible spin states in G . The Ising model associates to each vertex in Γ_N an energy :

$$\mathcal{E}_{\{S_i\}} = J \sum_{\langle i,j \rangle \in B} S_i S_j + h \sum_{i \in V} S_i, \quad (1)$$

with $J < 0$ (resp. > 0) favoring ferromagnetic (resp. antiferromagnetic) ordering. For sake of presentation, we shall mainly discuss here the Ising model regular case, with equal h and J terms for all sites and bonds. However,

most of what will be said below in the first part, with respect to the Hadamard Transform action, applies as well to disordered (spin glass) problems, and even to n -body interactions.

B. Coding graphs and interacting Hamiltonians into binary vectors

In general, a graph is rather faithfully described by its adjacency $N \times N$ matrix A , with $A_{ij} = 1$ whenever sites $(i, j) \in B$ and zero instead. But, especially for non-planar graphs, we may be interested in having a finer description, pointing onto higher dimensional cells of the graph (faces, polyhedra, polytopes, etc.). A simple generic binary vector $|G\rangle$ of size 2^N , in a space with basis $\mathcal{B} = \{0, 1\}^{\otimes N}$ fulfills this task in the following way : a basis vector is an ordered sequence of 0 and 1. Each binary digit position will correspond to a vertex of the graph; the occurrence of these different vertices in the graph is marked by a component 1 for the basis vectors having one 1 at the site position and $N - 1$ zeros elsewhere. A n -cell of the graph is a subset of n vertices; its presence in the graph is encoded in $|G\rangle$ as a component 1 for the basis vector having n terms equal to 1 at these vertices position and zero elsewhere.

The next step is to code the interacting n -body spin Hamiltonian as a coding vector $|C\rangle$. The interacting terms are associated to n -body cells : the external magnetic field acts onto one-body cells (vertices), the standard Ising interaction onto (two-body) edges, etc ... The vector $|C\rangle$ has non vanishing components, equal to the related n -body interaction term, precisely for those basis vector which code the corresponding n -body cell in $|G\rangle$. As a very simple example, a graph composed of two vertices joined by a bond will be characterized, in the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, by $|G\rangle = (0, 1, 1, 1)$, and its (Ising model) coding vector as $|C\rangle = (0, h_1, h_2, J_{1,2})$; the site position is ordered here from right to left, as in standard binary decomposition. Notice also that we are now switching from the above $(\pm 1)^{\otimes N}$ spin configuration notation to the equivalent $\{0, 1\}^{\otimes N}$ one with, say, an implicit bijection between $+1$ (or \uparrow) to the binary label 0.

III. ISING SPECTRUM FROM HADAMARD TRANSFORM

A. Hadamard Transform

We describe now how to simply compute these interacting spin models spectra, eventually leading to a natural speed up in their numerical derivation. The spectrum has M terms (therefore exponential with N), discretely ranging in an interval which generically grows linearly with N . It is therefore, as is well known, highly degenerate, in a way which cannot be solely captured by the graph G and global spin symmetries. We propose here to analyze this spectrum with tools analogous to the Fourier transformation, but adapted to the peculiar Γ_N hypercube geometry. This is precisely the task fulfilled by the so-called Hadamard transform (HT; one sometimes finds additional names associated to it, like Walsh and Rademacher), which is a linear transformation on a 2^N -dimensional space, given, with the standard basis $\{0, 1\}^{\otimes N}$, by the $2^N \times 2^N$ Hadamard matrix H_M defined recursively (with $H_0 = 1$) as

$$H_{m+1} = \begin{pmatrix} H_m & H_m \\ H_m & -H_m \end{pmatrix}; \text{ with } H_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \text{ and } H_2 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \quad (2)$$

A normalization factor $1/\sqrt{2}$ is often multiplied on the right-hand-side for H_1 , but will prove useful only in the second part of this presentation. The above relation reads also $H_{m+1} = H_1 \otimes H_m$; one easily also gets that $H_{p+q} = H_p \otimes H_q$. Hadamard matrices have the nice property that their rows or columns are pairwise orthogonal. The component $H_{p,q}$, with line p and row q both starting from zero, can be written in a compact way, by considering the base 2 decomposition p_j and q_j of p and q :

$$H_{p,q} = (-1)^{\sum p_j q_j} \quad (3)$$

B. The Hadamard transformed coding state

For a given spin configuration, each bond contributes through a term $\pm J$ to the energy, according to whether the two spins points to similar or opposite directions. In addition, each site contributes by $\pm h$ according to the local spin orientation. The complexity in computing the spectrum amounts to adding ‘‘coherently’’ these contributions for each

$\{S_i\}$ configuration. Coherent addition of amplitudes is precisely what the quantum framework knows how to deal with. This is why, although not a necessity, we shall adopt quantum-like notations to describe our proposed recipe.

Let us write the Ising Hamiltonian for quantum spins (in the S^z basis) with Pauli matrices instead of classical spins (only σ^x matrices are used, so no added quantum complications)

$$\mathcal{H} = J \sum_{\langle i,j \rangle \in B} \sigma_i^x \sigma_j^x + h \sum_{i \in V} \sigma_i^x \quad (4)$$

Let $|0\rangle$ be the fully polarized (which could be called here a vacuum state) in the initial standard σ^z basis. As easily checked, the above Ising coding state simply reads $|C\rangle = \mathcal{H} |0\rangle$.

We now define the spectral state $|E\rangle$ as the HT of $|C\rangle$: $|E\rangle = H_N |C\rangle$. The main first result of this paper states that $|E\rangle$ have components which are precisely the energies of the associated classical Ising model we started with, a point which can be understood by considering carefully how the above $H_{p,q}$ terms enters the matrix action in the Hadamard transformation. Notice that, interestingly, in the quantum spin context, this amounts to a basis change from the σ^z to the σ^x basis (a basis change precisely done by H_N , if the above mentioned normalization factor $1/\sqrt{2}$ is introduced). $|C\rangle$ is the superposition of an entangled bond vector $|B\rangle = J \sum_{\langle i,j \rangle \in B} \sigma_i^x \sigma_j^x |0\rangle$ and site vector $|S\rangle = h \sum_{i \in B} \sigma_i^x |0\rangle$. The HT of a given component, say $\sigma_i^x \sigma_j^x |0\rangle$, peaks out a factor ± 1 according to whether spins (i, j) are parallel or not (see expression (3)). The contributions are then added coherently, and the total amplitude is precisely the corresponding Ising classical energy.

Notice that the HT has already been mentioned in the context of spin glass Ising models⁵, but used quite differently. Here, the introduction of the spectral vector $|E\rangle$ as the HT of the coding state make its role direct and transparent.

To illustrate our approach, let us describe the simplest cases of two and three spins forming a bond and a triangle. With $N = 2$, the coding state has already been given above, and the spectral state reads

$$|E\rangle_2 = (2h + J, -J, -J, -2h + J) \quad (5)$$

whose components are indeed the classical Ising energies. With $N = 3$, the coding state reads $|C\rangle = (0, h, h, J, h, J, J, 0)$, which is transformed by H_3 to the Ising amplitudes

$$|E\rangle_3 = (3h + J, h - J, h - J, -h - J, h - J, -h - J, -h - J, -3h + J) \quad (6)$$

C. Discussion

We end this first part by a set of remarks :

1. Fast Hadamard Transform.

Even though interesting in itself, the present framework may not prove to be operational for spectrum determination, as compared to more straightforward enumerations, owing to the manipulation of large size Hadamard matrices. However a quite interesting feature arises from the existence of a FHT algorithm, widely used for instance in early digital image compression⁶, which therefore should provide ways to fasten the Ising spectrum computation for an arbitrary graph once the coding state is known. FHT relies upon the above iterative construction of H_{m+1} from H_1 and H_m , which iteratively “block diagonalizes” the transformation. Whether the use of FHT, combined with the sparseness of the coding vector (although not evident for the above two examples with two and three spins), would significantly speed up spectral computations, and at least compare to classical methods, is certainly worth being further checked. A simple way to deal with the sparseness of $|C\rangle$ is just to focus on those Hadamard matrix columns corresponding to the non vanishing elements of the coding states; such a column is readily computed as a tensor product of $(1, 1)$ and $(1, -1)$ column vectors, corresponding to the ordered occurrences of “0” or “1” in the binary decomposition of the column position (where, as for the derivation of expression 3, the first column start at position 0). In the case of regular graphs, as defined below, we will find a significant speed increase through the derivation of a recursive relation for the spectrum.

2. Extension to more complex models.

Up to now, we have concentrated on the regular Ising model model, with constant J and h parameters. However, inspection of expression 3 shows that the coherent addition of interaction contributions pertains for non regular

parameters. A spin glass-like coding state, where disorder affects either the local magnetic field or the couplings (or both) will also lead to the correct spectral state. Even more, as again can be checked from expression 3, generalized classical spin 1/2 models containing n-body interactions can be treated equally.

3. Experimental implementation.

As noted above, the HT operates a basis change from the σ^z to the σ^x basis. This opens the possibility for an interesting experimental implementation : first prepare the (generically) entangled coding state in the σ^z basis, and then measures this state in the x orientation. Recall however that the spectral state $|E\rangle$ has the Ising energies as “probability” amplitudes, which should be squared to compare with experimental occurrences (and therefore would not distinguish two energies opposite in sign). We do not claim here that this would give an operational method to compute large Ising models spectra. But, with an entangled coding state to be prepared, and quantum coherence to be achieved through the HT, it could already provide an interesting test for any quantum machine claiming to work in a quantum regime.

4. Transformation paths from the coding to the spectral state.

The standard Fourier transform relates a real and a dual reciprocal (or momentum) space. We see here that the HT (which can be viewed as a multidimensional discrete Fourier transform) relates a vector coding interactions on a graph to a (dual) vector coding the corresponding Ising energies. Suitably normalized, the HT is a unitary transformation; it is then rather tempting to follow continuously this transformation in spin space, ending at the full HT, and see what could be learned from this. Some preliminary attempts on small systems display interesting but complex patterns for the amplitudes and the degeneracies, but did not lead us to a clear or meaningful understanding of the coding state trajectory.

A different approach would consist in applying the H.T. spin after spin, following a discrete path to reach the full HT. In fact, a close inspection shows that it corresponds to the way the FHT algorithm works.

IV. ISING MODEL ON REGULAR STRUCTURES

By a regular structure we mean here a structure which can be built iteratively by adding identical substructures. A simple case is provided by an hypercube γ_d in dimension d , made of two γ_{d-1} (note that, hypercubes being ubiquitous here, we use “ γ ” for the structure, and “ Γ ” for the configuration space). We show now that, for such regular structures, the spectral state $|E\rangle$ can be computed iteratively in a rather efficient way, even compared to a direct use of a standard FHT. The demonstration will use some algebraic tools that are first recalled. Notice that the proposed framework also apply, as a one-step procedure, for line to line or plane to plane addition in a lattice and allows therefore for standard transfer matrix constructions, which are discussed in a second step.

A. Some definitions and notations

Let us first recall some linear algebra operations, and define related notations, that will prove useful below. All are elementary, but at the same time refer to sometimes unusual tools (at least for a physicist) like the matrix Hadamard product or vec-like operators.

We write \mathbb{I}_n the identity matrix of size n , $\mathbf{1}_n$ the $n \times n$ matrix made of 1, and $|\mathbf{1}_n\rangle$ the corresponding size n vector. For a vector $|X\rangle$, we define the diagonal matrix $D_{|X\rangle}$ whose component D_{jj} is the j^{th} component X_j .

1. Hadamard products

The matrix Hadamard product “ \circ ”, also called entry wise product, multiplies pairwise elements of two matrices to form a third one ($C = A \circ B$, such that $C_{ij} = A_{ij}B_{ij}$). We shall also use below a “vector Hadamard product” $|A\rangle \circ |B\rangle$ whose components are the pair-wise product of components, and a left (resp. right) Hadamard product of a vector and a matrix, which amounts to multiply the matrix i^{th} row (resp. column) by the i^{th} component of the

vector. Notice that, for a matrix M and vector $|A\rangle$ of same linear size,

$$|A\rangle \circ M = D_{|A\rangle}.M, \text{ and } M \circ |A\rangle = M.D_{|A\rangle} \quad (7)$$

Having in mind the usual function elementary expansion, we shall call $\overset{\circ}{\exp}$ the “Hadamard matrix exponential” whose effect is $\left(\overset{\circ}{\exp}A\right)_{ij} = \exp(A_{ij})$, and extend this definition to vectors. We shall eventually use the (trivial) relation :

$$\overset{\circ}{\exp}(|A\rangle + |B\rangle) = \overset{\circ}{\exp}(|A\rangle) \circ \overset{\circ}{\exp}(|B\rangle) \quad (8)$$

2. A “special” sum for matrices and vectors

We define special matrix and vector sums \uplus as⁷ :

$$\begin{cases} A \uplus B = A \otimes \mathbf{1}_n + \mathbf{1}_n \otimes B \\ |A\rangle \uplus |B\rangle = |A\rangle \otimes |\mathbf{1}\rangle + |\mathbf{1}\rangle \otimes |B\rangle, \end{cases} \quad (9)$$

where the subscript n (the vector size) has been omitted, and “ \otimes ” is the standard Kronecker product. Be careful not to confuse with the standard matrix Kronecker sum $A \oplus B = A \otimes \mathbb{I}_n + \mathbb{I}_n \otimes B$ where the identity matrix \mathbb{I}_n appears instead the “one matrix” $\mathbf{1}$. Notice the useful relation :

$$\overset{\circ}{\exp}(A \uplus B) = \overset{\circ}{\exp}A \otimes \overset{\circ}{\exp}B, \quad (10)$$

which reminds (but differs from) the better known $\exp(A \oplus B) = \exp A \otimes \exp B$ involving the standard matrix exponential and Kronecker matrix sum.

3. The vec operator

The *vec* operator maps a $n \times m$ matrix onto a column vector of size $n * m$, simply built by stacking the successive columns of the original matrix. We are mainly interested here by square matrices, and would like also to use the inverse of a *vec* map, unraveling a vector of size n^2 onto an $n \times n$ matrix with its successive columns taken from the vector components. There is an apparent notation conflict here, some authors calling *devec* this operator, while others⁸ use *devec* to denote the operator building a row vector of size $n * m$ from the original matrix by concatenation of its successive rows. Therefore we shall adopt here the notation *unvec* for the inverse of *vec*. The following useful identity, involving three matrices P , Q and R will be used later:

$$\text{vec}(P.Q.R) = (R^T \otimes P).\text{vec}(Q), \quad (11)$$

where R^T is the matrix transpose of R , and the “dot” refers to the standard product for matrix algebra (between two matrices or a matrix and a vector).

B. The hypercube case

We now discuss a recursive algorithm to compute the Ising model spectra for the family of hypercubes with increasing dimensionality. Notice that, interestingly, a hypercube γ_{2d} is topologically equivalent to an hypercubic lattice of lateral size four in dimension d , with periodic boundary conditions (PBCs), noted here Z_d^4 . The latter inherits the former symmetry group, of order $(2d)!2^{2d}$. The hypercube γ_d has $N = 2^d$ sites; its spin configuration space is the hypercube Γ_M with $M = 2^N$. The recursive additive construction $\gamma_{d+1} = \gamma_d \cup T(\gamma_d)$, where $T(\gamma_d)$ is a translated version of γ_d in the new space dimension, leads to a Kronecker product for the respective configuration space : $\Gamma_{M^2} = \Gamma_M \otimes \Gamma_M$.

1. Ising addition spectrum for two uncorrelated subgraphs

Let us start by trivially writing the spectral vector for the union of two graphs G_1 and G_2 , both with N sites for sake of simplicity, but with possibly different interaction coding states (Ising model parameters). Compute first (say through FHT) the two spectral states $|E_1\rangle$ and $|E_2\rangle$. If the two graphs have no interactions, the spectral state of their union G , noted $|E\rangle$, is simply the “addition spectrum” of its two parts, an object which is precisely given by the above defined special vector sum $\uplus : |E\rangle = |E_1\rangle \uplus |E_2\rangle$.

The latter expression can be easily checked directly; let us nevertheless derive it in the present framework. Call $|0\rangle_N$ the fully polarized state with N spins, and $|C_1\rangle$ and $|C_2\rangle$ the coding states associated to G_1 and G_2 . Since up to now the latter are not Ising connected, the coding state for G simply reads

$$|C\rangle = |C_2\rangle \otimes |0\rangle_N + |0\rangle_N \otimes |C_1\rangle. \quad (12)$$

$|0\rangle_N$ is the first element in the standard basis $\{0,1\}^{\otimes N}$, and its HT is easily shown to be $|1\rangle_N$. As a result, the spectral state $|E\rangle$ reads

$$|E\rangle = H_{2N} \cdot |C\rangle = (H_N \otimes H_N) \cdot |C\rangle = |E_2\rangle \otimes |1\rangle_N + |1\rangle_N \otimes |E_1\rangle = |E_2\rangle \uplus |E_1\rangle \quad (13)$$

Now really interesting questions start when the graphs union is dressed with new couplings between the parts, with the task of combining coherently these new interactions with the simple “disconnected” addition spectrum.

2. Introducing interactions between the subgraphs

There are clearly three types of Ising (bond) interactions : those associated separately to G_1 or G_2 , and those connecting the two graphs. For reasons which will be clear below, we choose to consider the matrix $C_{2N} = \text{unvec}(|C_{2N}\rangle)$. The first two types of bonds appear in its first column as the column vector $|C_1\rangle$, and in its first row as the line vector $\langle C_2|$, a direct consequence of the above uncorrelated graph coding state in formula (12). The remaining part, forming a matrix D , codes the remaining interactions. It has non vanishing elements only at positions corresponding to an interacting bond between the graphs G_1 and G_2 . At this stage, this description is still generic and applies to the union of two different graphs, with possibly non regular bonding between the two graphs, the complexity being coded in D . We now show that for the class of regular graphs to which hypercubes belong, D takes a simple form which allow for a recursive analysis.

3. Ising spectrum for the hypercube

The additive construction of hypercubes translates into a simple iterative construction for the coding state vector from $|C_N\rangle$ to $|C_{2N}\rangle$. If we are cautious enough to number the sites coherently for the two γ_d copies (which means sites j and $j+N$ are translation related), we get a rather simple form for the matrix D which turns into a pure diagonal matrix, the third type of bonds contributions sitting at location $2^j + 1$ along the diagonal, with integer j running from 0 to $N-1$, and being simply related to the above defined site vector $|S_N\rangle$ associated to γ_d : $D_{2N} = J D_{|S_N\rangle}$.

To clarify our notations, let us display these objects for the easiest case, from the point γ_0 to the segment γ_1 and then to the square γ_2 :

$$|C_1\rangle = \begin{pmatrix} 0 \\ h \end{pmatrix}, |C_2\rangle = \begin{pmatrix} 0 \\ h \\ h \\ J \end{pmatrix}, C_2 = \begin{pmatrix} 0 & h \\ h & J \end{pmatrix}, D_2 = \begin{pmatrix} 0 & 0 \\ 0 & J \end{pmatrix}, C_4 = \begin{pmatrix} 0 & h & h & J \\ h & J & 0 & 0 \\ h & 0 & J & 0 \\ J & 0 & 0 & 0 \end{pmatrix}, D_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & J & 0 & 0 \\ 0 & 0 & J & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (14)$$

We aim to compute the Ising spectrum vector $|E_{2N}\rangle = H_{2N} |C_{2N}\rangle$. This could be done easily using FHT as discussed above. But we proceed differently here, by recalling that $H_{2N} = H_N \otimes H_N$ and that $H_N^T = H_N$. We then use relation (11), with $P = R = H_N$ and the above defined C_{2N} to get :

$$|E_{2N}\rangle = \text{vec}(H_N \cdot C_{2N} \cdot H_N) \quad (15)$$

This only difficult part requires now to evaluate a set of matrices $M_{2N} = H_N \cdot D_{2N} \cdot H_N$, the Hadamard transformed D_{2N} matrices, which happens to follow a simple iterative construction. Some easy algebra leads to the following coupled system, which iteratively constructs the hypercube Ising spectrum in any dimension :

$$\begin{cases} |E_{2N} > &= (|E_N > \uplus |E_N >) + \text{vec}(M_{2N}) \\ M_{2N} &= M_N \uplus M_N \end{cases} \quad (16)$$

As already said, the first term on the RHS of the first equation provides the expected addition spectrum from the two copies of γ_n , while the second term contains their interaction. We leave as an exercise to the interested reader to recover, from the initial $|E_1 > = (h, -h)$ and $M_2 = \text{unvec}(J, -J, -J, J)$, the Ising spectrum for a square :

$$|E_4 > = (4h + 4J, 2h, 2h, 0, 2h, 0, -4J, -2h, 2h, -4J, 0, -2h, 0, -2h, -2h, -4h + 4J) \quad (17)$$

Relation (16) is very easily iterated numerically. As an example, two additional iterations leads, almost instantaneously on a standard computer, to $|E_{16} >$, the spectrum for γ_4 , and therefore for the 4×4 square lattice system with periodic boundary conditions. It reads, with $J = 1$ and $h = 0$, given in frequency (pairs of numbers, first term for the energy, and second term its degeneracy) :

$$\{(-32, 2), (-24, 32), (-20, 64), (-16, 424), (-12, 1728), (-8, 6688), (-4, 13568), (0, 20524), \dots\} \quad (18)$$

We omit the positive part of the spectrum, the latter being symmetrical. Notice however that iterating relation (16) involves consecutive tensor products, which is paid for in terms of computer memory. If the γ_5 spectrum (which corresponds to a piece of cubic lattice of size $4 \times 4 \times 2$) is still very quickly computed, higher sizes turn out to be difficult to reach along this direct track, if equipped only with standard computers memory.

4. Partition function

We now aim to evaluate the partition function

$$\mathcal{Z} = \sum_{\{S_i\}} \exp(-\beta \mathcal{E}_{\{S_i\}}), \quad (19)$$

from which all interesting thermodynamical properties can be derived. The reader who has followed the present approach might have already guessed that we shall define a partition function vector $|Z >$ as :

$$|Z > = \exp^{\circ}(-\beta |E >) \quad (20)$$

where we use the above defined matrix Hadamard exponential. The standard \mathcal{Z} is simply the sum of $|Z >$ components. It is again not difficult to derive an iterative relation to get $|Z_{2N} >$ from $|Z_N >$, equivalent to expression (16) we had for the spectrum. With the diagonal matrix $D_{|Z\rangle}$ built from Z_N and $W_N = \exp^{\circ}(-\beta M_N)$, it reads

$$\begin{cases} |Z_{2N} > &= D_{|Z\rangle}^{\otimes 2} \cdot \text{vec}(W_{2N}) = \text{vec}(D_{|Z\rangle} \cdot W_{2N} \cdot D_{|Z\rangle}) \\ W_{2N} &= W_N \otimes W_N \end{cases} \quad (21)$$

Although quite simple, we detail, in Appendix A, the step by step passage from relation (16) to relation (21). The second line of relation 21 arises directly from that of relation 16 upon using relation (10). Quite interestingly, upon additional manipulations, the partition function itself, \mathcal{Z}_{2N} , which is the sum of all $|Z_{2N} >$ elements, simply reads

$$\mathcal{Z}_{2N} = \langle Z_N | W_{2N} | Z_N \rangle \quad (22)$$

Let us stress that the present approach is different from that followed in Ref.⁹, where the partition function \mathcal{Z} was computed as the inner product of a stabilizer state and a product state, and for the sake of which these authors defined spins living on edges of the graph. In the present case, the square partition function \mathcal{Z}_4 is computed as, with $x = \exp(-\beta J)$,

$$\mathcal{Z}_4 = (x, x^{-1}, x^{-1}, x) \begin{pmatrix} x^2 & 1 & 1 & x^{-2} \\ 1 & x^2 & x^{-2} & 1 \\ 1 & x^{-2} & x^2 & 1 \\ x^{-2} & 1 & 1 & x^2 \end{pmatrix} \begin{pmatrix} x \\ x^{-1} \\ x^{-1} \\ x \end{pmatrix} = 2(6 + x^4 + x^{-4}) \quad (23)$$

An interesting point arises here. The matrix W_N , which encodes the coupling between the two sub parts, is diagonalized by a Hadamard matrix (now normalized to have unitary transformations). Indeed, start with the first in the series,

$$W_2 = \begin{pmatrix} x & x^{-1} \\ x^{-1} & x \end{pmatrix} \quad (24)$$

It is diagonalized under transformation by H_1 :

$$W'_2 = H_1 \cdot W_2 \cdot H_1 = \begin{pmatrix} x + x^{-1} & 0 \\ 0 & x - x^{-1} \end{pmatrix} \quad \text{with now } H_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (25)$$

Due to the simple tensor product construction of W_N , explicit in the second line of (21), together with the tensor product construction for the Hadamard matrices, the spectrum of W_N is computed directly from that of W_2 . Recalling that Hadamard matrices square to identity, we can insert the identity matrix on the left and on the right of W_{2N} in expression (22). This leads to an expression for the partition function as the expectation value of the (known) diagonalized form of W_{2N} , taken on the HT of the partition function of the sub parts $|Z_N\rangle$. For the square case, expression (23) now rewrites :

$$\mathcal{Z}_4 = (x + x^{-1}, 0, 0, x - x^{-1}) \begin{pmatrix} x^2 + x^{-2} + 2 & 0 & 0 & 0 \\ 0 & x^2 - x^{-2} & 0 & 0 \\ 0 & 0 & x^2 - x^{-2} & 0 \\ 0 & 0 & 0 & x^2 + x^{-2} - 2 \end{pmatrix} \begin{pmatrix} x + x^{-1} \\ 0 \\ 0 \\ x - x^{-1} \end{pmatrix} = 2(6 + x^4 + x^{-4}) \quad (26)$$

Notice that for the case of two-dimensional grids, and without disorder, there are powerful methods to derive partition functions for large but finite size systems¹⁰.

C. Transfer matrices

As already mentioned, the above step by step treatment for the hypercubes also applies, as a one-step procedure, to describe line to line or plane to plane (or graph to graph) addition to form a repeated structure in a given direction. Call Λ_N the graph with N vertices to be repeated, and $\Lambda_{2N} = \Lambda_N \cup T(\Lambda_N)$ the resulting graph after one step. We consider the simplest case where each vertex in Λ_N has one (translated) neighbor in $T(\Lambda_N)$, suitably numbered as before. The case where each vertex has several new neighbors in the translated copy (as occurs for instance in dense lattices like fcc) could also be treated, with some complications, and will not be analyzed here. With $|E_N\rangle$ and $|Z_N\rangle$ for the Ising spectrum and partition vector for the Λ part, relations (16) and (21) still apply to get $|E_{2N}\rangle$ and $|Z_{2N}\rangle$. But, more interestingly, and as expected, the transfer matrix itself is easily derived. T_N , the $2^N \times 2^N$ transfer matrix from Λ_N to $T(\Lambda_N)$, simply reads :

$$T_N = W_{2N} \cdot D_{|Z\rangle} = W_{2N} \circ |Z_N\rangle \quad (27)$$

With m copies of Λ (and periodic boundary condition), the partition function follows from the well known trace relation $\mathcal{Z}_{mN} = \text{Tr}(T_N^m)$.

While a full diagonalization of T would solve the problem, we shall ask, more modestly, whether Hadamard transformations (with normalized Hadamard matrices from now on) can be helpful to further simplify T_N , under the form of a partial block-diagonalization. A simple first step, but nevertheless rather trivial, consists in operating a global HT to the transfer matrix; notice that one should better say an Hadamard conjugation since it reads : $T \rightarrow H^{-1} \cdot T \cdot H$. This leads to split the transfer matrix into two separate blocks, which in fact translates the existence of a global spin-flip symmetry. One could then try to go further and operate with lower order Hadamard matrices on the two blocks. First attempts on small systems show that it might be the case, although no precise conclusions could yet be drawn. As an example, we detail the process in Appendix B for the 16×16 transfer matrix T_4 connecting two rings of four spins, which we analyze here in the vanishing h magnetic field limit, and for which a partial block diagonalization has been achieved.

V. CONCLUSION

We have presented a general framework to address Ising-like models on arbitrary graphs. The interactions between spins are neither limited to pairwise interactions, nor restricted to constant couplings. The present approach relies on

a dual structure : a coding state on one side, which represents the interactions carried by the spins, is transformed into a spectral state whose amplitudes are the model energies. The transformation is operated by Hadamard matrices.

A interesting point here is the existence of a FHT, which provides therefore potential for speed increase for numerical computation, in particular if sparse vectors manipulations are cleverly introduced. Whether FHT, sparse algebra and parallelism could be efficiently associated here is an open question that may interest numerical experts.

When the graph is obtained as the union of subgraphs, the proposed analysis simply separates the contribution of the sub graph spectra from that arising from their interaction. Whenever the interaction takes a regular form, we have shown how to compute iteratively the spectrum.

Attempts to compute the partition function and transfer matrices have also been described. Further works need to be done, in particular to check possible transfer matrix block diagonalization algorithms.

In addition, the fact that the HT is a main tool for quantum computation raises the question of a possible experimental implementation of the proposed approach.

Finally, one may ask whether this type of approach could be used for other collective models, like higher spins systems or the Potts model. However, using standard Hadamard matrices (with +1 and -1 entries), combined with the above defined coding vector, restricts the application to spins carrying only two distinct values (with symmetric interactions), therefore to Ising spins only.

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VI. APPENDIX

A. Derivation of the partition function vector $|Z\rangle$ in expression 21

As said above, it is not difficult to derive an iterative relation to get $|Z_{2N}\rangle$ from $|Z_N\rangle$, given in expression 21. It provides nevertheless an interesting exercise to manipulate some of the algebraic tools introduced in the text, and we therefore detail it now, step by step:

$$\begin{aligned}
|Z_{2N}\rangle &\stackrel{def}{=} \exp(-\beta |E_{2N}\rangle) \\
&= \exp[-\beta (|E_N\rangle \uplus |E_N\rangle) - \beta \text{vec}(M_{2N})] \\
&= \exp[-\beta (|E_N\rangle \uplus |E_N\rangle)] \circ \exp[-\beta \text{vec}(M_{2N})] \quad \text{from (8)} \\
&= [\exp(-\beta |E_N\rangle) \otimes \exp(-\beta |E_N\rangle)] \circ \text{vec}\left(\exp(-\beta M_{2N})\right) \quad \text{from (10) and obvious vec/exp commutation} \\
&= |Z_N\rangle^{\otimes 2} \circ \text{vec}(W_{2N}) \\
&= D_Z^{\otimes 2} \cdot \text{vec}(W_{2N}) \quad \text{from (8) (Q.E.D.)} \\
&= \text{vec}(D_Z \cdot W_{2N} \cdot D_Z) \quad \text{from (11)}
\end{aligned}$$

The second line of relation 21 arises directly from that of relation 16 upon using relation (10)

B. Partial block diagonalization of the transfer matrix: A simple example.

As announced in the text, we present here the case of the 16×16 transfer matrix T_4 connecting two rings of four spins, which is analysed in the vanishing h magnetic field limit. Notice that this simple example is just meant here to introduce a proposition which clearly need to be further checked for larger cases. Using relations 21 and 27, one easily writes T_4 as :

$$T_4 = \begin{pmatrix} x^8 & x^6 & x^6 & x^4 & x^6 & x^4 & x^4 & x^2 & x^6 & x^4 & x^4 & x^2 & x^4 & x^2 & x^2 & 1 \\ x^2 & x^4 & 1 & x^2 & 1 & x^2 & \frac{1}{x^2} & 1 & 1 & x^2 & \frac{1}{x^2} & 1 & \frac{1}{x^2} & 1 & \frac{1}{x^4} & \frac{1}{x^2} \\ x^2 & 1 & x^4 & x^2 & 1 & \frac{1}{x^2} & x^2 & 1 & 1 & \frac{1}{x^2} & x^2 & 1 & \frac{1}{x^2} & \frac{1}{x^4} & 1 & \frac{1}{x^2} \\ 1 & x^2 & x^2 & x^4 & \frac{1}{x^2} & 1 & 1 & x^2 & \frac{1}{x^2} & 1 & 1 & x^2 & \frac{1}{x^4} & \frac{1}{x^2} & \frac{1}{x^2} & 1 \\ x^2 & 1 & 1 & \frac{1}{x^2} & x^4 & x^2 & x^2 & 1 & 1 & \frac{1}{x^2} & \frac{1}{x^2} & \frac{1}{x^4} & x^2 & 1 & 1 & \frac{1}{x^2} \\ 1 & x^2 & \frac{1}{x^2} & 1 & x^2 & x^4 & 1 & x^2 & \frac{1}{x^2} & 1 & \frac{1}{x^2} & \frac{1}{x^4} & 1 & x^2 & \frac{1}{x^2} & 1 \\ \frac{1}{x^4} & \frac{1}{x^6} & \frac{1}{x^2} & \frac{1}{x^4} & \frac{1}{x^2} & \frac{1}{x^4} & 1 & \frac{1}{x^2} & \frac{1}{x^6} & \frac{1}{x^2} & \frac{1}{x^4} & \frac{1}{x^6} & \frac{1}{x^4} & \frac{1}{x^6} & \frac{1}{x^2} & \frac{1}{x^4} \\ \frac{1}{x^2} & 1 & 1 & x^2 & 1 & x^2 & x^2 & x^4 & \frac{1}{x^2} & \frac{1}{x^2} & \frac{1}{x^4} & x^2 & 1 & 1 & 1 & x^2 \\ x^2 & 1 & 1 & \frac{1}{x^2} & 1 & \frac{1}{x^2} & \frac{1}{x^2} & \frac{1}{x^4} & x^2 & x^2 & 1 & x^2 & 1 & 1 & 1 & \frac{1}{x^2} \\ \frac{1}{x^4} & \frac{1}{x^2} & \frac{1}{x^6} & \frac{1}{x^4} & \frac{1}{x^2} & \frac{1}{x^4} & \frac{1}{x^2} & \frac{1}{x^4} & \frac{1}{x^2} & 1 & \frac{1}{x^4} & \frac{1}{x^2} & \frac{1}{x^4} & \frac{1}{x^2} & \frac{1}{x^6} & \frac{1}{x^4} \\ 1 & \frac{1}{x^2} & \frac{1}{x^6} & x^2 & 1 & \frac{1}{x^2} & \frac{1}{x^4} & 1 & \frac{1}{x^2} & 1 & x^4 & x^2 & 1 & \frac{1}{x^2} & x^2 & 1 \\ \frac{1}{x^2} & 1 & 1 & x^2 & \frac{1}{x^2} & \frac{1}{x^4} & \frac{1}{x^2} & 1 & 1 & x^2 & x^2 & x^4 & \frac{1}{x^2} & 1 & 1 & x^2 \\ 1 & \frac{1}{x^2} & \frac{1}{x^2} & \frac{1}{x^4} & x^2 & 1 & 1 & \frac{1}{x^2} & x^2 & 1 & 1 & \frac{1}{x^2} & x^4 & x^2 & x^2 & 1 \\ \frac{1}{x^2} & 1 & \frac{1}{x^4} & \frac{1}{x^2} & 1 & x^2 & \frac{1}{x^2} & 1 & 1 & x^2 & \frac{1}{x^2} & 1 & x^2 & x^4 & 1 & x^2 \\ \frac{1}{x^2} & \frac{1}{x^4} & 1 & \frac{1}{x^2} & 1 & \frac{1}{x^2} & x^2 & 1 & 1 & \frac{1}{x^2} & x^2 & 1 & x^2 & 1 & x^4 & x^2 \\ 1 & x^2 & x^2 & x^4 & x^2 & x^4 & x^4 & x^6 & x^2 & x^4 & x^4 & x^6 & x^4 & x^6 & x^6 & x^8 \end{pmatrix} \quad (28)$$

A first (trivial) block-diagonalization (two 8×8 blocks), associated with the global spin-flip symmetry, is provided by transforming T_4 to $H_4.T_4.H_4$ (recall that $H_4 = H_4^{-1}$ in the normalized case). Combining suitable columns and row permutations, and Hadamard matrices of lower order, one then gets the following spectrum for T_4 : a set of eight eigenvalues, shown as pairs (eigenvalue, degeneracy d): $\{(x^4 - 2 + x^{-4}, d = 4), ((1 + x^2)(x^2 - 1)^3/x^4, d = 2), ((1 + x^2)^3(x^2 - 1)/x^4, d = 2)\}$; the following two 2×2 matrices :

$$\begin{pmatrix} x^8 - 1 & 2x^2(x^4 - 1) \\ \frac{2(x^4 - 1)}{x^2} & \frac{x^8 - 1}{x^4} \end{pmatrix}, \text{ and } \begin{pmatrix} 1 - x^{-8} & \frac{2(x^4 - 1)}{x^6} \\ \frac{2(x^4 - 1)}{x^2} & \frac{1 - x^{-8}}{x^4} \end{pmatrix}, \quad (29)$$

and one 4×4 matrix :

$$\begin{pmatrix} x^8 + 1 & 2x^4 & \sqrt{2}(x^2 + \sqrt{2}x^4 + x^6) & \sqrt{2}(-x^2 + \sqrt{2}x^4 - x^6) \\ 2x^{-4} & x^{-8} + 1 & \frac{\sqrt{2}(x^2 + \sqrt{2}x^4 + x^6)}{x^8} & \frac{\sqrt{2}(-x^2 + \sqrt{2}x^4 - x^6)}{x^8} \\ 2 + \frac{\sqrt{2}(1+x^2)}{x^4} & 2 + \frac{\sqrt{2}(1+x^2)}{x^4} & x^{-4} + 2\sqrt{2}x^{-2} + 4 + 2\sqrt{2}x^2 + x^4 & -2 \\ 2 - \frac{\sqrt{2}(1+x^2)}{x^4} & 2 - \frac{\sqrt{2}(1+x^2)}{x^4} & -2 & x^{-4} - 2\sqrt{2}x^{-2} + 4 - 2\sqrt{2}x^2 + x^4 \end{pmatrix} \quad (30)$$

These small matrices could again be further simplified, but (apparently) not with HTs, so we do not show it. The interested reader can easily recover, from $Tr(T_4^4)$, the partition function for a 4×4 square lattice with PBC, whose Ising spectrum was already given in relation (18).